CompassCDS
Column and Solvent Database Plug-in
User Guide

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Using the Column and Solvent Database Plug-in

This document describes the functions of the Column and Solvent Database Plug-in for CompassCDS.

Overview

The Column and Solvent Database Plug-in enables users to manage columns and solvents that are used in chromatographic systems. The columns and solvents and their properties are defined in a database that is available from CompassCDS. The Column and Solvent database is used for all chromatography types.

The Column and Solvent Database Plug-in permits users to automatically increment column parameters at each system injection. The Generic Column Tracker driver must be added as part of the configured system in CompassCDS and a column from the list must be selected in the method.

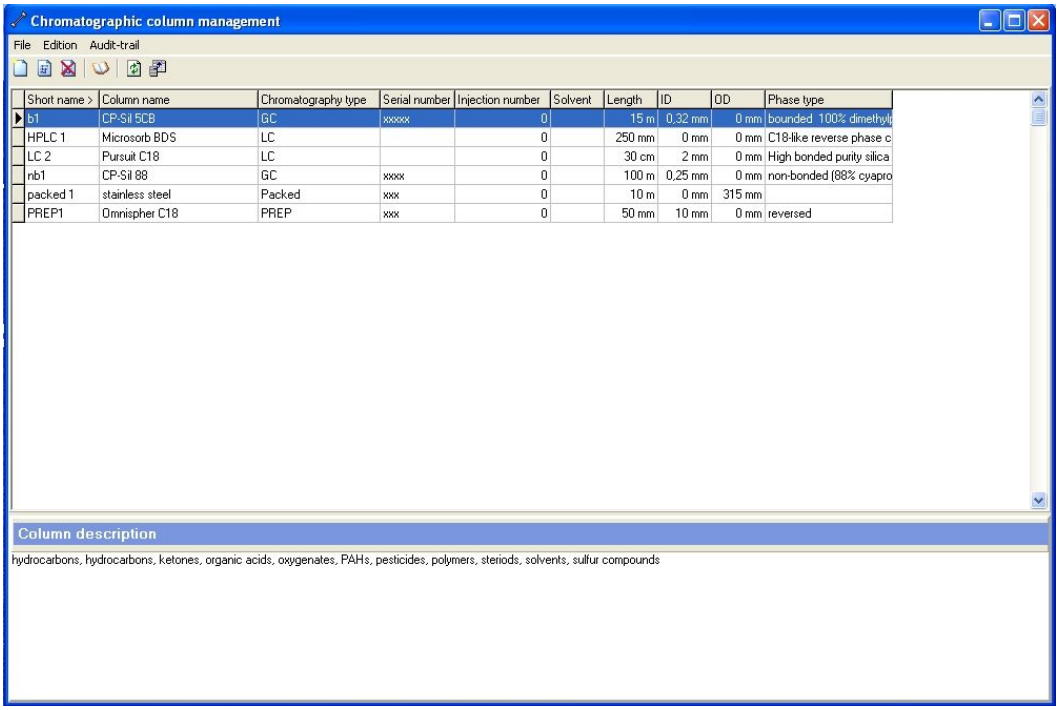
This plug-in can also manage solvent miscibility for Column Valve Modules.

A common audit trail lists all modifications in columns and solvents properties. The audit trail, the column and solvent properties and lists are exportable and printable.

Software functions

Chromatographic Column Management

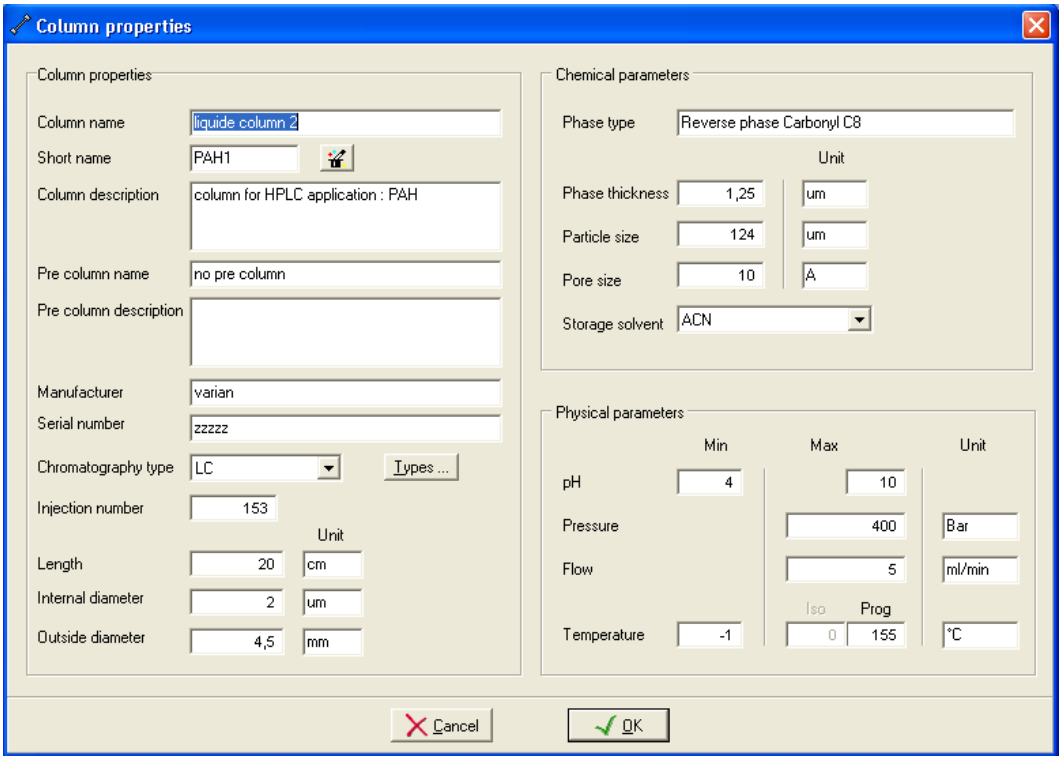
In CompassCDS, open the Chromatographic column management by selecting the icon or the corresponding option in the Plug-ins menu. The following screen is displayed:


Chromatographic column management
File Edition Audit-trail
Short name > Column name Chromatography type Serial number Injection number Solvent Length ID OD Phase type
b1 CP-Sil 5CB GC xxxxx 0 15 m 0,32 mm 0 mm bounded 100% dimethyl
HPLC 1 Microsorb BDS LC 0 250 mm 0 mm 0 mm C18-like reverse phase c
LC 2 Pursuit C18 LC 0 30 cm 2 mm 0 mm High bonded purity silica
nb1 CP-Sil 88 GC xxxx 0 100 m 0,25 mm 0 mm non-bonded (88% cyapro
packed 1 stainless steel Packed xxx 0 10 m 0 mm 315 mm
PREP1 Omnispher C18 PREP xxx 0 50 mm 10 mm 0 mm reversed
Column description
hydrocarbons, hydrocarbons, ketones, organic acids, oxygenates, PAHs, pesticides, polymers, steriods, solvents, sulfur compounds

It contains the list of all defined columns of the database. When selecting a column line, the Column description is displayed at the bottom of the screen.

Adding a New Column and Modifying Column Parameters

Define a new column in the column database by pressing the button, selecting ***EDITION / NEW*** menu or in the contextual menu. Modify the properties of a selected column by pressing, double-clicking, selecting EDITION / EDIT or in the contextual menu. Enter or modify the column parameters in the displayed column properties screen:



Only the column short name field need be completed, and all other fields are optional.

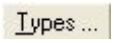
Validate the new settings by clicking on or cancel these.

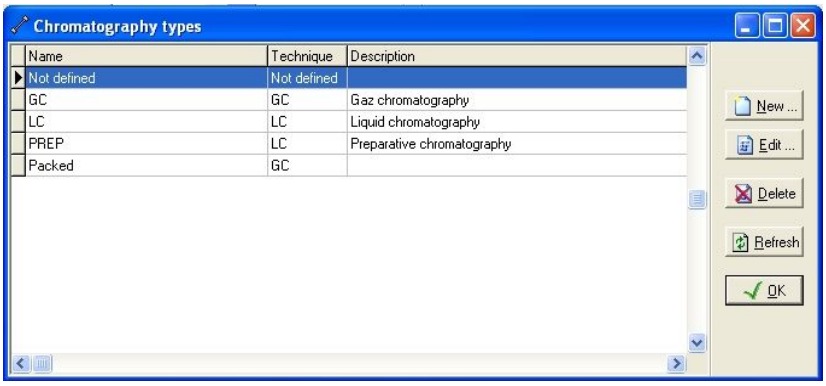
Column Properties Parameter Group

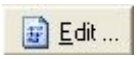
In the Column name field, enter the entire column name.

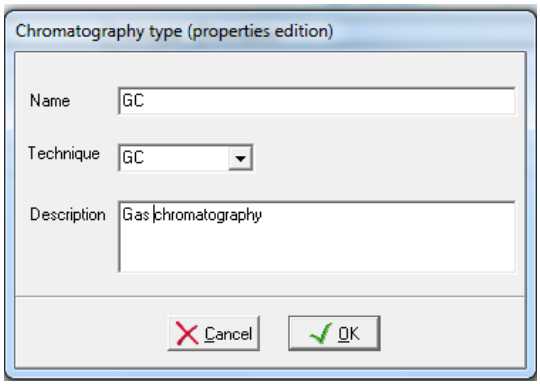
In the Short name field, enter a short name or click on the button to automatically define the 10 first characters of the Column name as Short name. The Short name is used for the CompassCDS column identification within a method and is mandatory.

Fill in the Column description, the Pre column name, the Pre column description, the Manufacturer name and the Serial number of the column.

Select the Chromatography type in the corresponding scrolling list. By default, GC, LC, PREP, Packed and Not defined are the available types. Press  to modify the chromatography types list. The following screen is displayed:



Press to add a new chromatography type and press  to modify the selected one. Choose the Technique and fill in the new Description and Name field in the displayed Chromatography type properties edition screen:



Validate the new settings by clicking on .

Press to delete the selected chromatography type and to refresh the list.

Fill in the column Length, Internal diameter, outside diameter and units in the corresponding fields.

Chemical Parameters Parameter Group

Enter the Phase type, Film thickness, Particle size, Pore size and units in the corresponding fields. Choose the Storage solvent among the whole Solvent database list.

Note that the Particle size, Pore size and Storage solvent fields are only available when the Chromatography technique is LC.

Physical Parameters Parameter Group

Enter the pH minimum and maximum values tolerated by the column in the Min and Max fields.

Enter the maximum Pressure and Flow with the units that the column can stand.

It is possible to fill in the pH and Flow fields only when the chromatography technique is LC.

Enter the column minimum and maximum temperatures when used in isothermal or programmed mode.

Managing the Columns List

Delete a selected column of the list by selecting the button, selecting EDITION / DELETE menu or from the contextual menu.

To duplicate a column entry in the list, select it and then the EDITION / DUPLICATE menu or from the contextual menu. A new column entry is created with exactly the same parameters except the Column name and the Short name. The column name of the created column entry begins with “copy of” and ends with the name of the duplicated column entry. The Short name of the created column entry corresponds to the first 9 characters of the duplicated Column name ended by a number suffix.

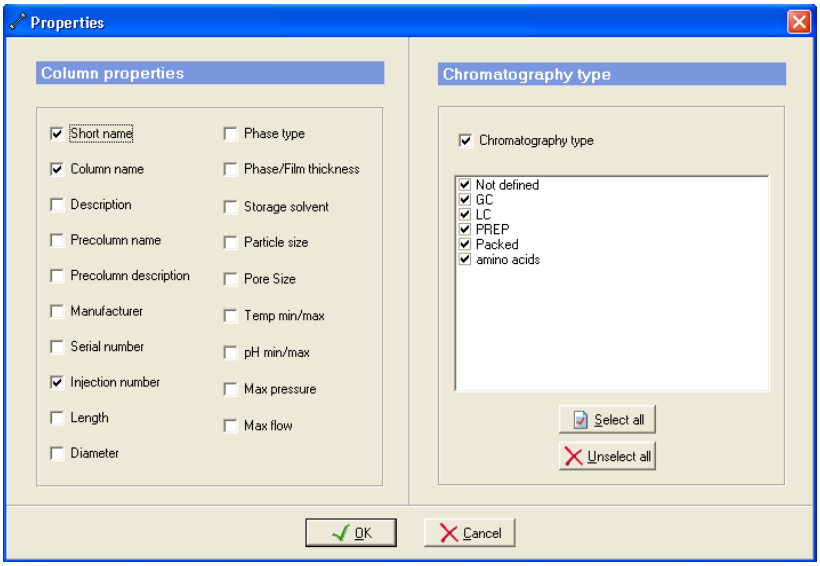
Print or Export in HTML the columns list by selecting EDITION / PRINT LIST or EDITION / EXPORT LIST. Choose the path to export and the file is automatically displayed at screen. The column parameters that are printed and exported are the currently displayed in the table and the Column description.

Print or Export in HTML each column parameters by selecting EDITION / PRINT PROPERTIES or EDITION / EXPORT PROPERTIES or from the contextual menu. Choose the path to export and the file is automatically displayed at screen.

Displaying Column Parameters

Click on the button to refresh the database as this can be modified from different stations at the same time, when in Client/Server configuration.

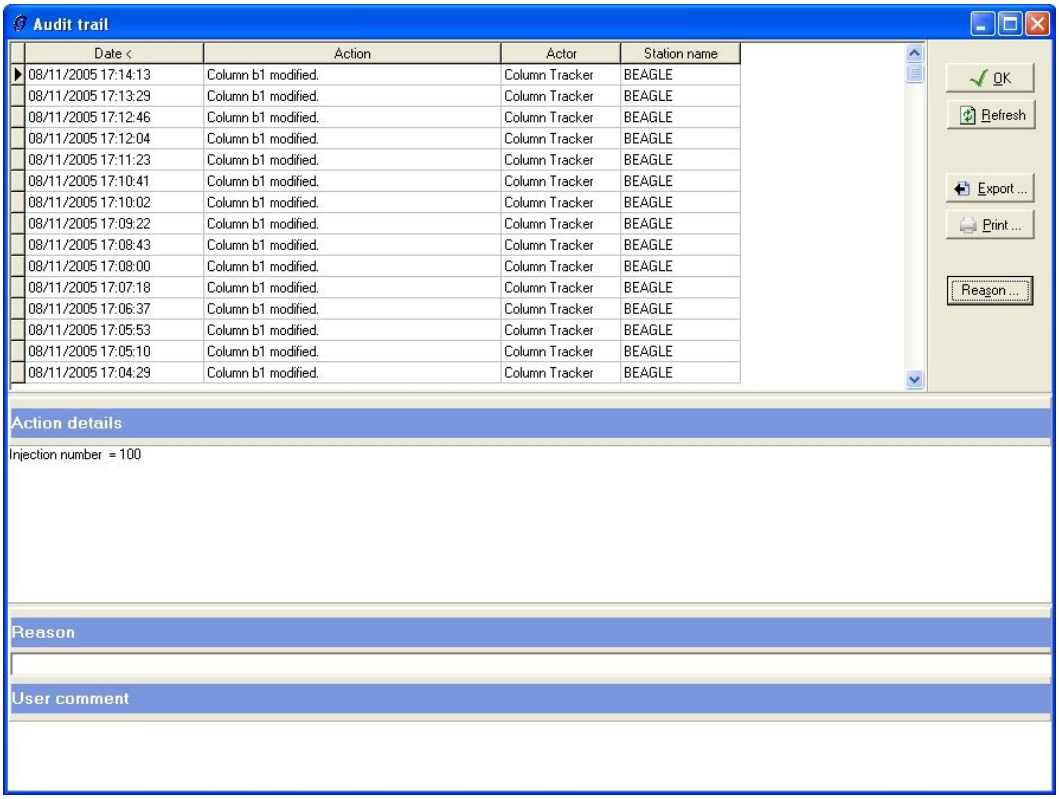
Click on the button or select Properties in the contextual menu to change the parameters to display in the column table. The following screen is then displayed:



To display a parameter in the column list table, check the corresponding box in the Column properties part. To display particular columns in the list depending on the type of chromatography, select that type in the Chromatography type section. Press Select all or Unselect all to select all available chromatography types or to unselect all checked types.

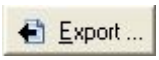
Displaying Column and Solvent Database Audit Trail

Press the button or select the AUDIT TRAIL / VIEW AUDIT TRAIL menu to display the column and solvent database audit trail.


Audit trail
Date <
Action
Actor
Station name
08/11/2005 17:14:13 Column b1 modified. Column Tracker BEAGLE
08/11/2005 17:13:29 Column b1 modified. Column Tracker BEAGLE
08/11/2005 17:12:46 Column b1 modified. Column Tracker BEAGLE
08/11/2005 17:12:04 Column b1 modified. Column Tracker BEAGLE
08/11/2005 17:11:23 Column b1 modified. Column Tracker BEAGLE
08/11/2005 17:10:41 Column b1 modified. Column Tracker BEAGLE
08/11/2005 17:10:02 Column b1 modified. Column Tracker BEAGLE
08/11/2005 17:09:22 Column b1 modified. Column Tracker BEAGLE
08/11/2005 17:08:43 Column b1 modified. Column Tracker BEAGLE
08/11/2005 17:08:00 Column b1 modified. Column Tracker BEAGLE
08/11/2005 17:07:18 Column b1 modified. Column Tracker BEAGLE
08/11/2005 17:06:37 Column b1 modified. Column Tracker BEAGLE
08/11/2005 17:05:53 Column b1 modified. Column Tracker BEAGLE
08/11/2005 17:05:10 Column b1 modified. Column Tracker BEAGLE
08/11/2005 17:04:29 Column b1 modified. Column Tracker BEAGLE
OK
Refresh
Export ...
Print ...
Reason ...
Action details
Injection number = 100
Reason
User comment

All modifications in the column parameters are listed in the audit trail with the corresponding date, actor and station. Each time an acquisition is done using a column that is defined in the Column and Solvent Database and in a system using the column tracker driver, the injection number of the column is automatically incremented in the column parameters. In that case, the actor listed in the audit trail is the name of the system and the system acquisition server is listed as station name.

Click on the button to refresh the audit trail.

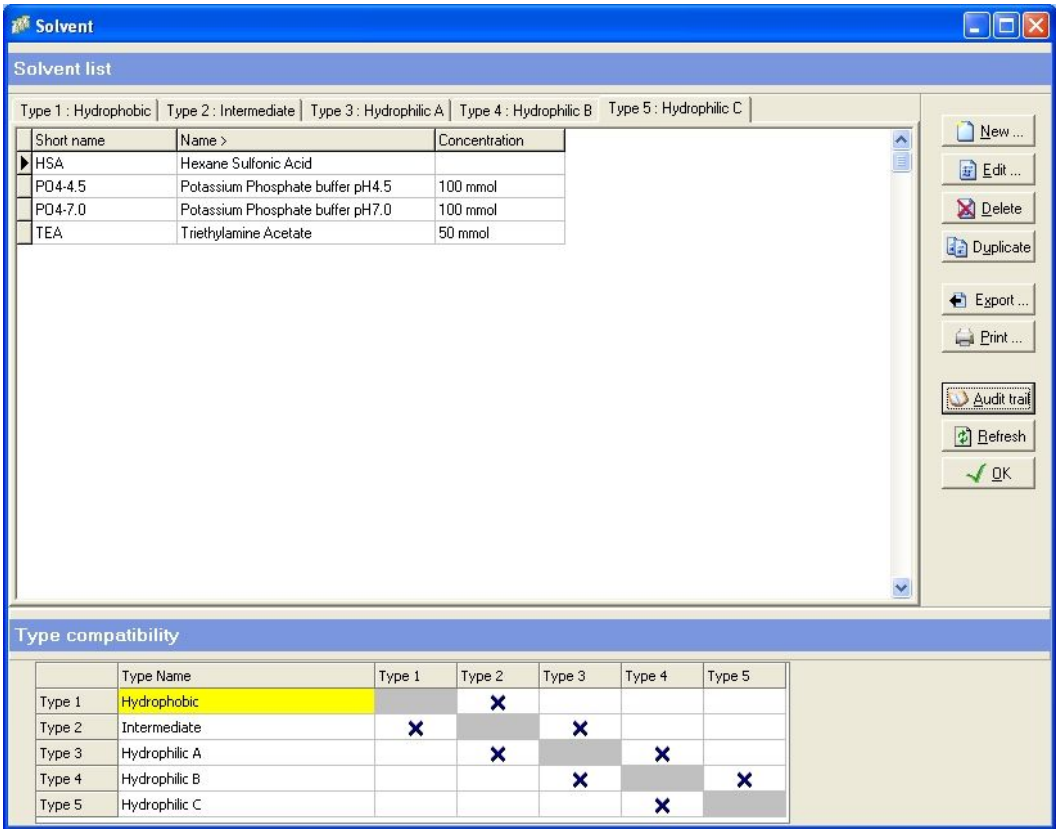
Click on the  button to export the current audit trail. Choose the export folder path and the file is automatically displayed at screen.

Click on the button to print the current audit trail.

Press the button to display user reasons and comments.

Chromatographic Solvent Management

In CompassCDS, open the Chromatographic Solvent Management by selecting the icon or the corresponding option in the Plug-ins menu. The following screen is displayed:

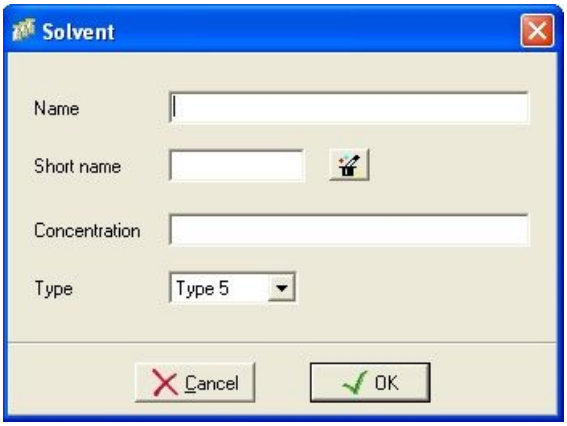


It contains the list of all defined solvents that are distributed into 5 different tabs depending on their hydrophobicity or hydrophilicity. Hydrophilic solvents are dispensed into three different types: the more hydrophilic corresponds to Type 5, the less hydrophilic to Type 3 and the moderately well hydrophilic to Type 4. The hydrophobic solvents are listed in the Type 1 tab and the solvents of intermediate hydrophobia in the Type 2 tab.

At the bottom of the screen, the Type compatibility table indicates the miscibility between solvents of different solvent types.

Adding a New Solvent and Modifying Solvent Parameters

Define a new solvent in the solvent type database by pressing the New ... button or from the contextual menu. Modify the properties of a selected solvent by pressing Edit ... or from the contextual menu. Enter or modify the solvent parameters in the displayed column properties screen:



Enter the solvent Name and Concentration.

In the Short name field, enter a short name or click on the button to automatically define the 10 first characters of the solvent name as Short name. The Short name is used for the CompassCDS solvent identification.

The solvent Name and Short name must be filled in.

Managing the Solvents List

Delete a selected solvent entry of the list by pressing the Delete button or from the contextual menu.

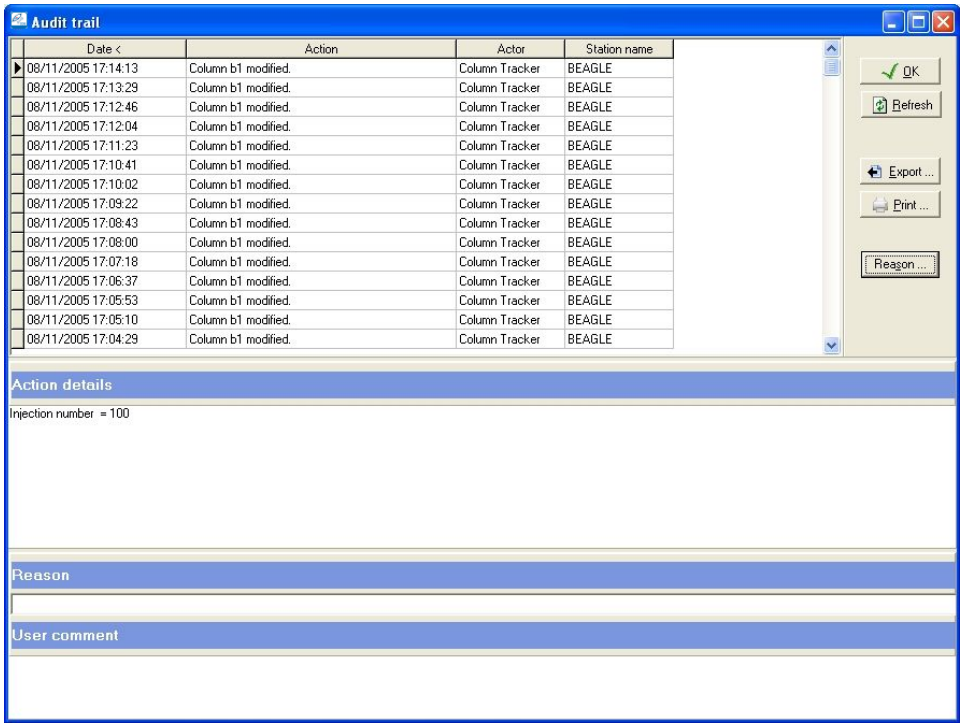
To duplicate a selected solvent entry in the list, press Duplicate or select it from the contextual menu. A new solvent entry is created with exactly the same parameters except the solvent *Name* and the *Short name*. The solvent *Name* of the created solvent entry begins with “copy of” and ends with the name of the duplicated solvent entry. The *Short name* of the created solvent entry corresponds to the first 9 characters of the duplicated solvent name ended by a number suffix.

Print or Export the solvent list and parameters by pressing the Print ... or Export ... button. Choose the path to export and the file is automatically displayed at screen.

Click on the Refresh button to refresh the database that can be modified from different stations at the same time, when in Client/Server configuration.

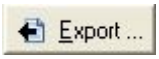
Displaying Solvents and Columns Database Audit Trail

Press the Audit trail button to display the column and solvent database audit trail.


Audit trail
Date <
Action
Actor
Station name
08/11/2005 17:14:13 Column b1 modified. Column Tracker BEAGLE
08/11/2005 17:13:29 Column b1 modified. Column Tracker BEAGLE
08/11/2005 17:12:46 Column b1 modified. Column Tracker BEAGLE
08/11/2005 17:12:04 Column b1 modified. Column Tracker BEAGLE
08/11/2005 17:11:23 Column b1 modified. Column Tracker BEAGLE
08/11/2005 17:10:41 Column b1 modified. Column Tracker BEAGLE
08/11/2005 17:10:02 Column b1 modified. Column Tracker BEAGLE
08/11/2005 17:09:22 Column b1 modified. Column Tracker BEAGLE
08/11/2005 17:08:43 Column b1 modified. Column Tracker BEAGLE
08/11/2005 17:08:00 Column b1 modified. Column Tracker BEAGLE
08/11/2005 17:07:18 Column b1 modified. Column Tracker BEAGLE
08/11/2005 17:06:37 Column b1 modified. Column Tracker BEAGLE
08/11/2005 17:05:53 Column b1 modified. Column Tracker BEAGLE
08/11/2005 17:05:10 Column b1 modified. Column Tracker BEAGLE
08/11/2005 17:04:29 Column b1 modified. Column Tracker BEAGLE
OK
Refresh
Export ...
Print ...
Reason ...
Action details
Injection number = 100
Reason
User comment

All modifications in the solvent parameters are listed in the audit trail with the corresponding date, actor and station.

Click on the button to refresh the audit trail.

Click on the  button to export the current audit trail. Choose the path to export and the file is automatically displayed at screen.

Click on the button to print the current audit trail.

Press the button to display user reasons and comments.

Using the Generic Column Tracker Driver

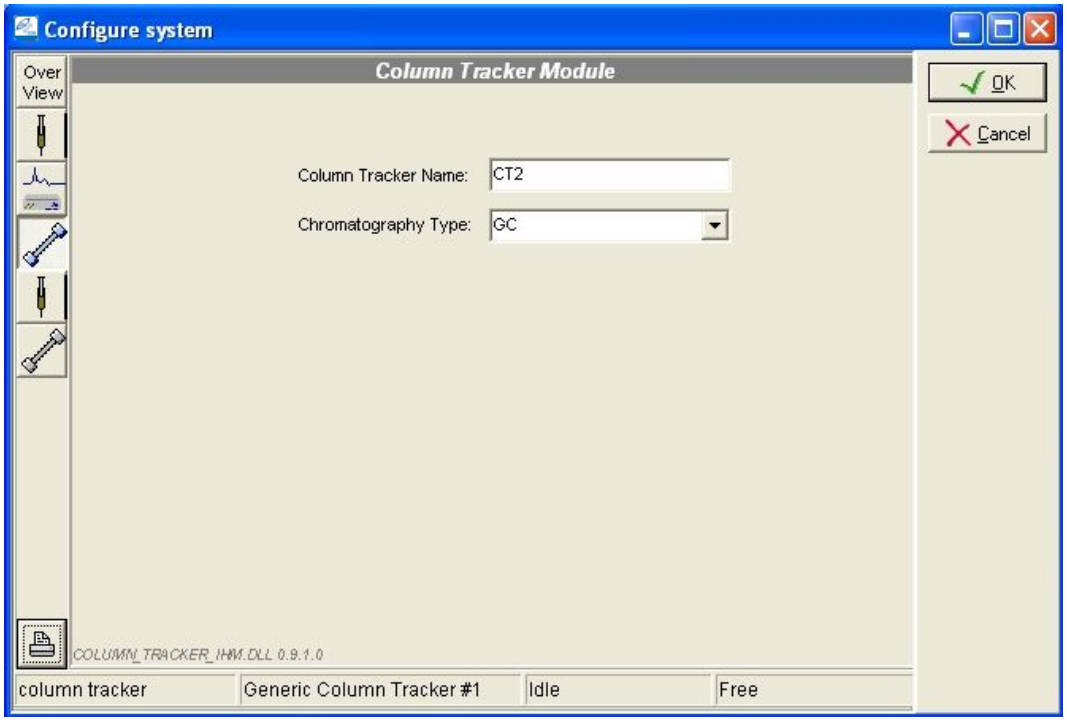
Use the Generic Column Tracker Driver in order to use the Column and Solvent Management Plug-in to automatically increment column parameters.

Configuring the Generic Column Tracker

The driver software configuration is done in the CompassCDS Configuration Manager when a new chromatographic system is created.

NOTE: If the system is equipped with several columns, it is necessary that system driver list contains an equivalent number of instances of the column tracker driver as there are columns in the system.

Click on the button corresponding to the Generic Column Tracker driver and the configuration screen appears.



In cases where the system contains several columns, enter a Column Tracker Name to differentiate each column. This Column Tracker Name should be different for each Column tracker module of the system.

Choose the Chromatography Type of each column of the system in the corresponding scrolling list. All the defined chromatography types of the column database are available.

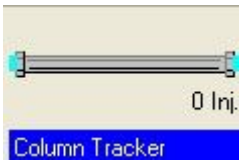
Configuring the Synopsis

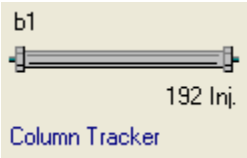
In the Overview part of the system configuration, a synopsis can be defined for the system. This synopsis depends on the configured devices.

Right click on the system name in the bottom part of the CompassCDS Configuration Manager screen. A pop-up menu appears: click on Stop. Then right click on the system name again, and click on Start.

The synopsis will be displayed in CompassCDS in the Systems tab. In this tab, the Overview will show the synopsis of the system.

For example, the following pictures represent the synopsis of the Generic Column Tracker:





NOTE: Once the system has been created and correctly configured, it must be associated with one or more projects in order to start some acquisitions. For more details about the creation and configuration of a system, refer to the CompassCDS Configuration Manager User Guide.

Press the button to print the current configuration.

Building a Method

Create a new method for the system using the Generic Column Tracker driver.

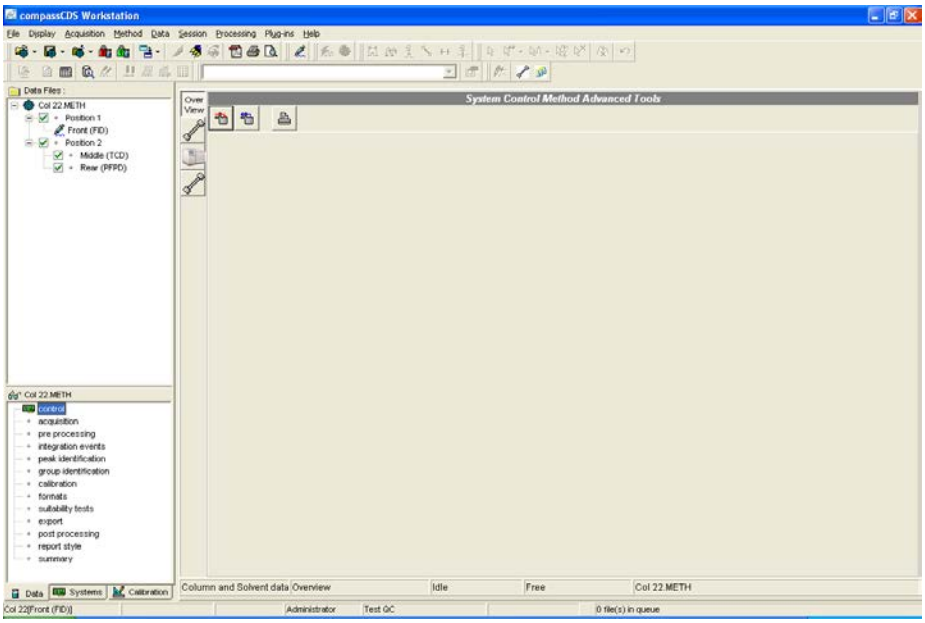
The control section must be defined in order to start an acquisition. In the following part of this guide, only the control section for the Generic Column Tracker is described.

NOTE: For more details about the programming of each method section, consult the CompassCDS User Guide.

Control Method Section for the Generic Column Tracker

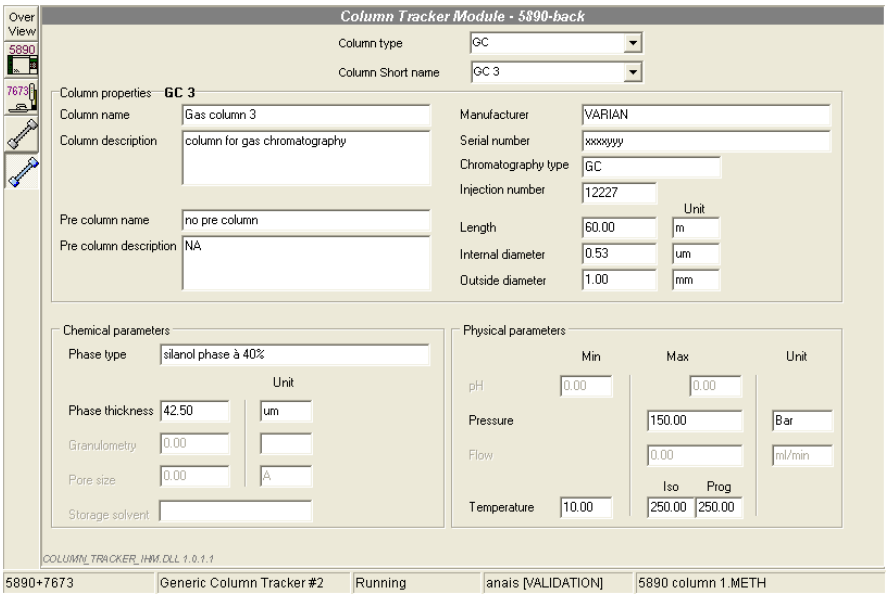
In the method, select the control section in the lower part of the browser.

The following screen appears:



Click on the button to display the Generic Column Tracker control method section.

Column Tracker Module Control



The Chromatography type chosen while configuring the system is displayed at the top of the control screen.

Select the Column Short name to be used in the system in the corresponding scrolling list just above. Only the columns defined for this Chromatography type are available in the scrolling list.

Once a column is selected, its Column properties, Chemical parameters and Physical parameters are automatically displayed on screen.

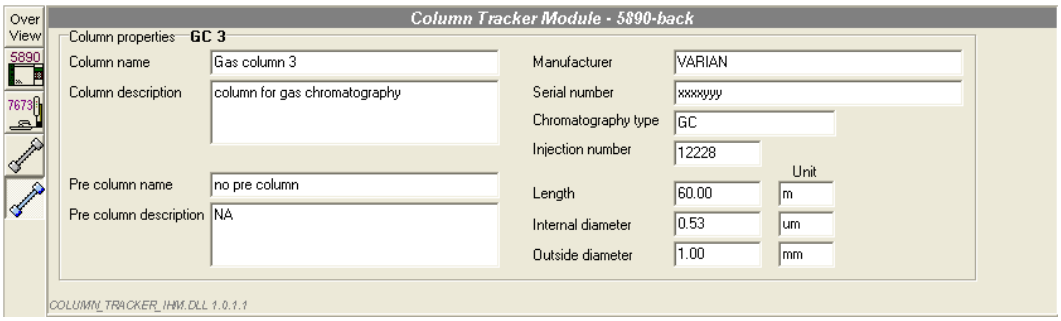
Starting and Viewing an Acquisition

To view a running acquisition, click on the Systems tab then select the running system.

Status of the Generic Column Tracker

Click on the button corresponding to the Generic Column Tracker driver and the Generic Column Tracker status screen will appear.

Status Window



The Status window displays the column properties as defined in the column database. All fields are in read-only mode. The Injection number is incremented at each injection.